Functional Data Analysis in a Nutshell

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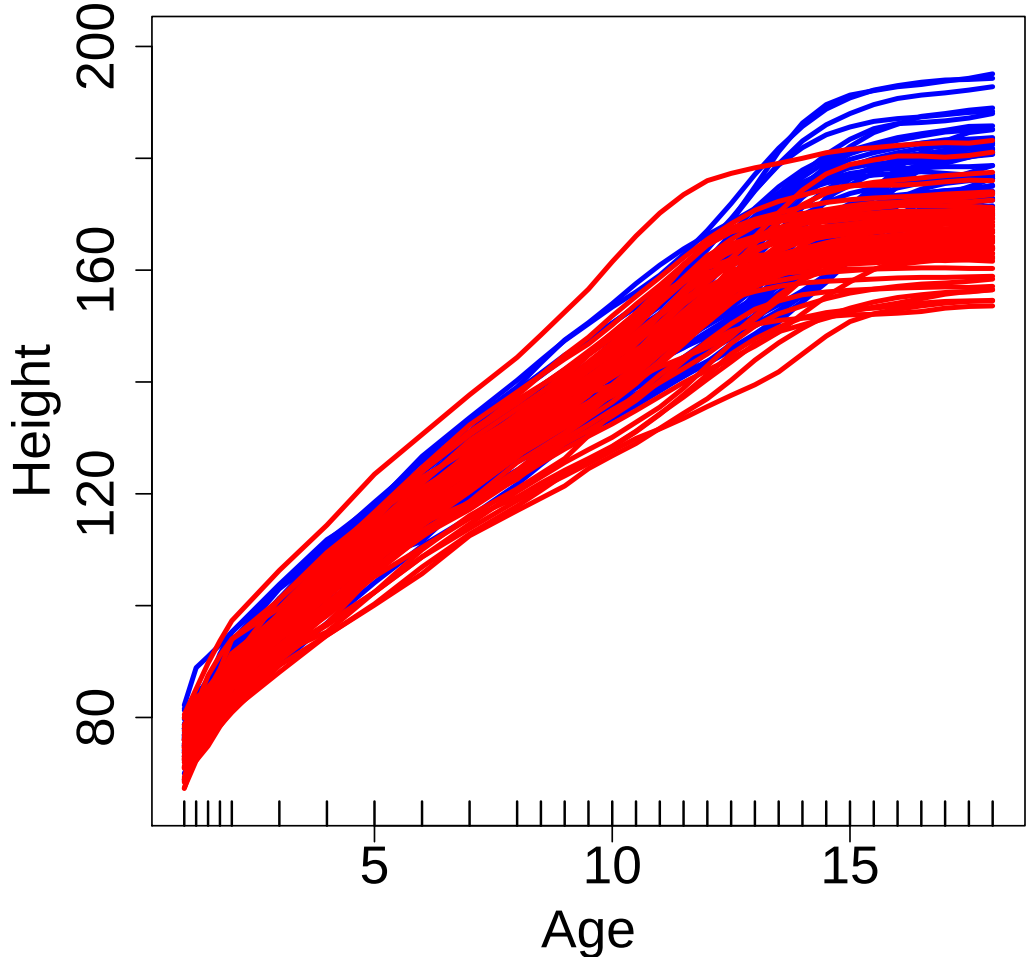
Introduction to functional data



(Ramsay & Silverman, 2005)

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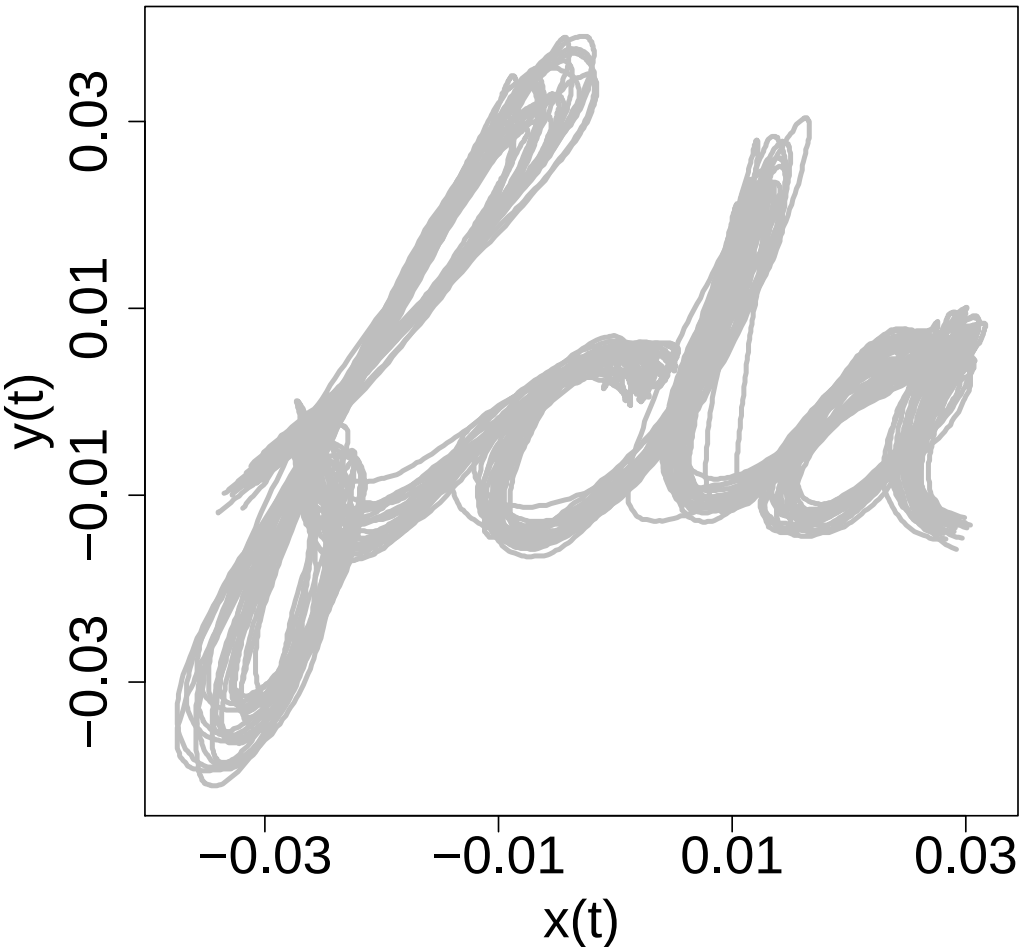

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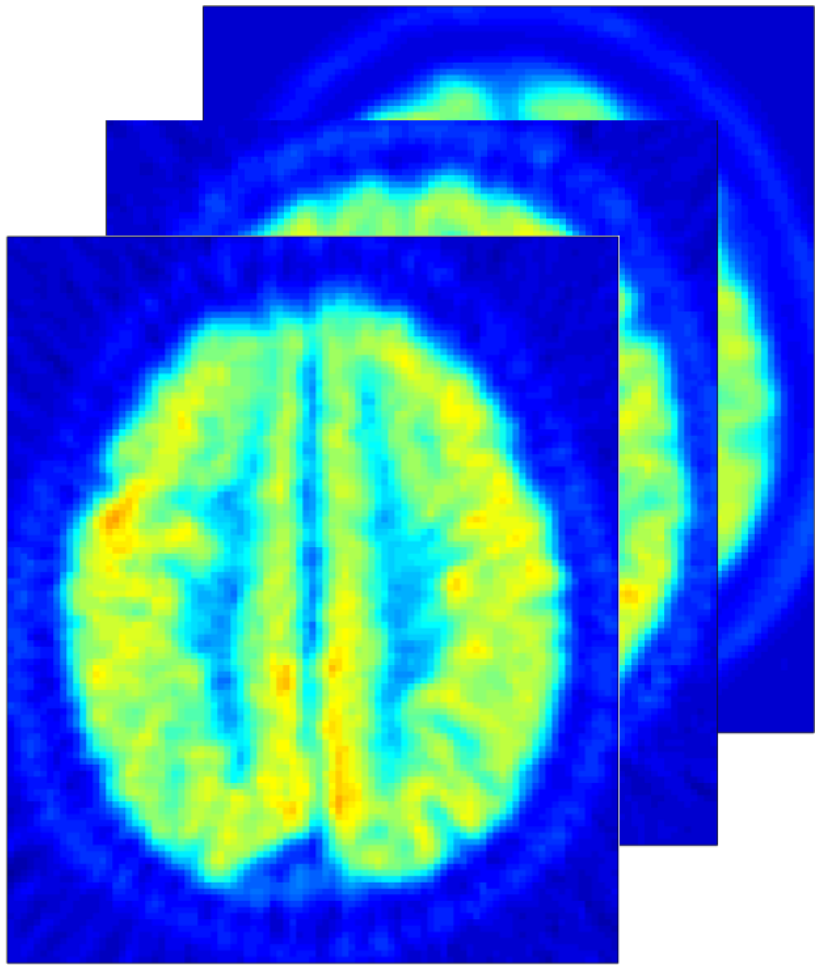

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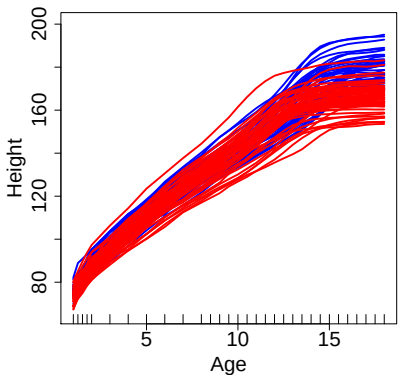

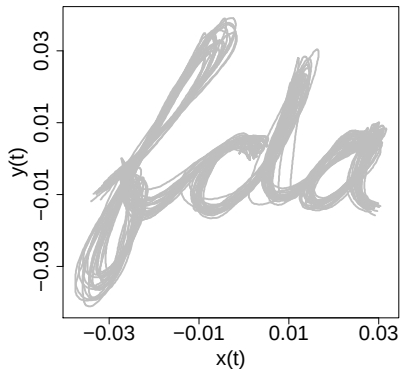

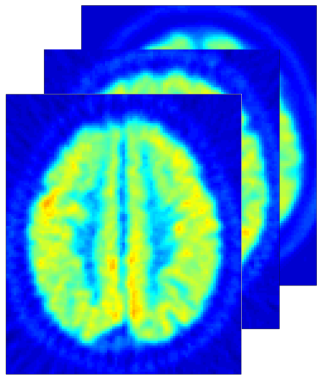

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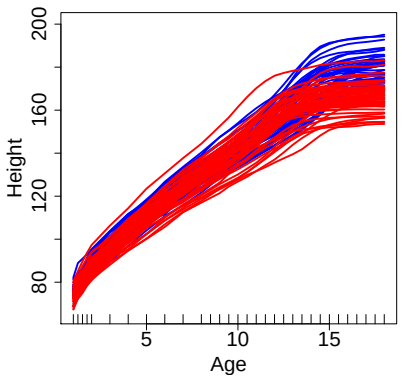

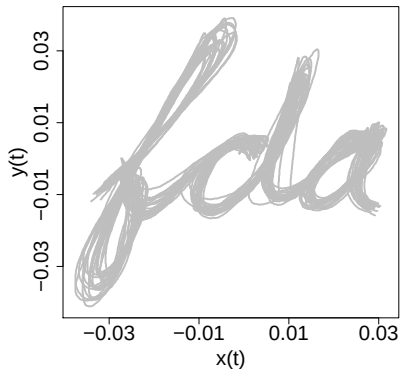

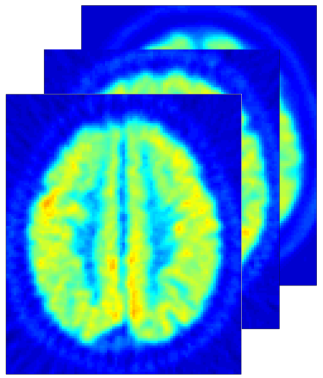

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- Measures on regular or irregular grids, sparse or dense data

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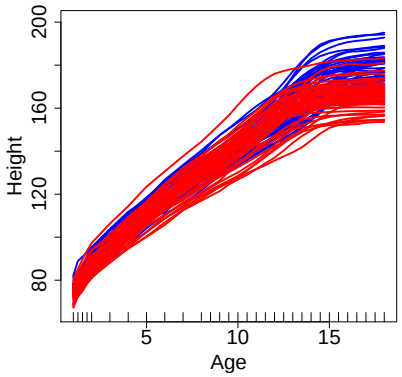

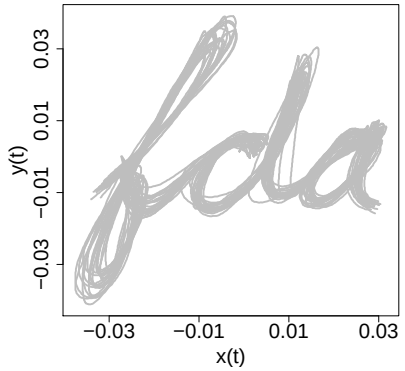

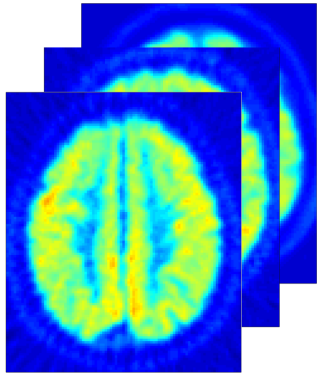

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- Possibly arbitrary many measurements possible
  $\rightarrow$ smooth data generating function

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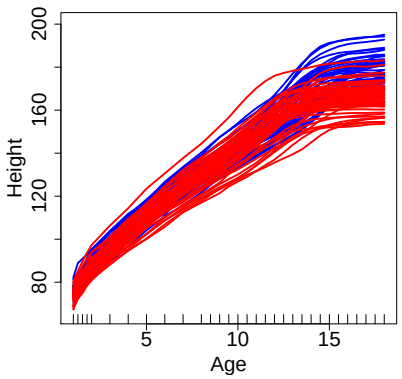

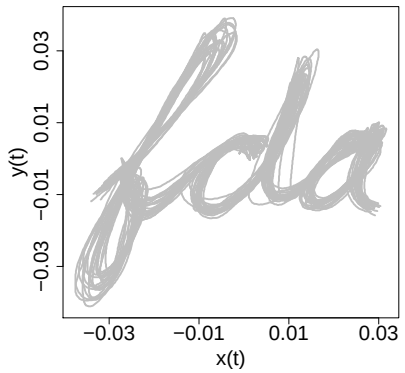

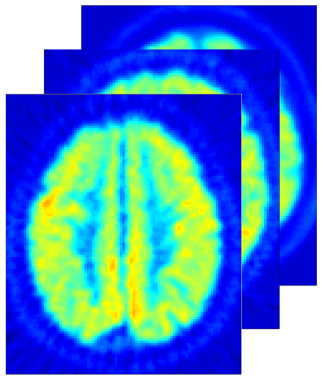

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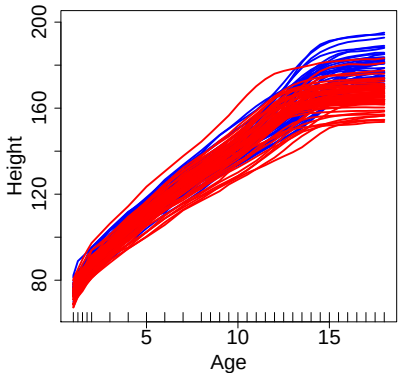

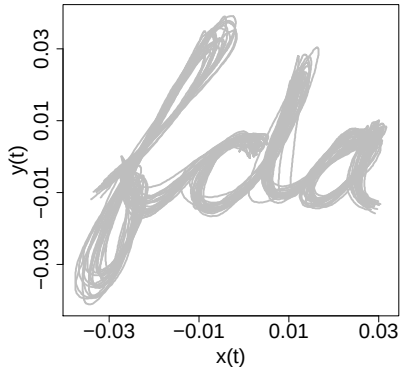

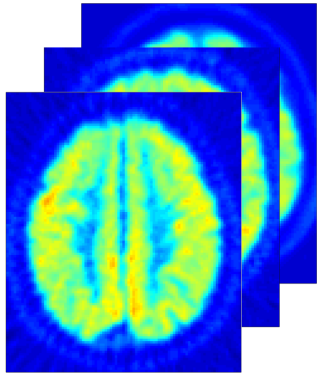

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- Measures on regular or irregular grids, sparse or dense data
- Possibly arbitrary many measurements possible
  $\rightarrow$ smooth data generating function
- Observations possibly with (measurement) error
- Many observations of the same data generating process and no prediction for further observations in the future
  $\leftrightarrow$ time series analysis

Progress of statistics

progress of mathematical statistics in terms of:

- sample space X: where the available data live
- parameter space Θ: where the target parameter belongs
- sample size n, number of variables d and number of parameters k

Statistical theory	**sample space X**	**parameter space Θ**
Classical parametric inference	$\mathbb{R}$	$\Theta \subset \mathbb{R}$
Multivariate analysis	$\mathbb{R}^d$ $(n \gg d)$	$\Theta \subset \mathbb{R}^k$ $(n \gg k)$
Nonparametrics	$\mathbb{R}^d$ $(n \gg d)$	a function space
High dimensional problems	$\mathbb{R}^d (n < d)$	$\Theta \subset \mathbb{R}^k$
Functional data analysis	a function space	$\mathbb{R}^k$ / a function space

(Cuevas, 2014)

Basic statistics for functional data

Mean, Variance and Covariance

- functional variable $X(t)$,
  with $t \in \mathcal{T}$ and $\mathcal{T}$ interval in $\mathbb{R}$
- sample $x_i(t)$, $i = 1, \ldots, n$

Mean, Variance and Covariance

- functional variable $X(t)$,
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- sample $x_i(t)$, $i = 1, \ldots, n$
- functional mean:

$$\hat{\mu}_X(t) = \bar{x}(t) = \frac{1}{n} \sum_{i=1}^{n} x_i(t)$$

- functional variance:

$$\hat{\sigma}_X(t) = \frac{1}{n-1} \sum_{i=1}^{n} [x_i(t) - \bar{x}(t)]^2$$

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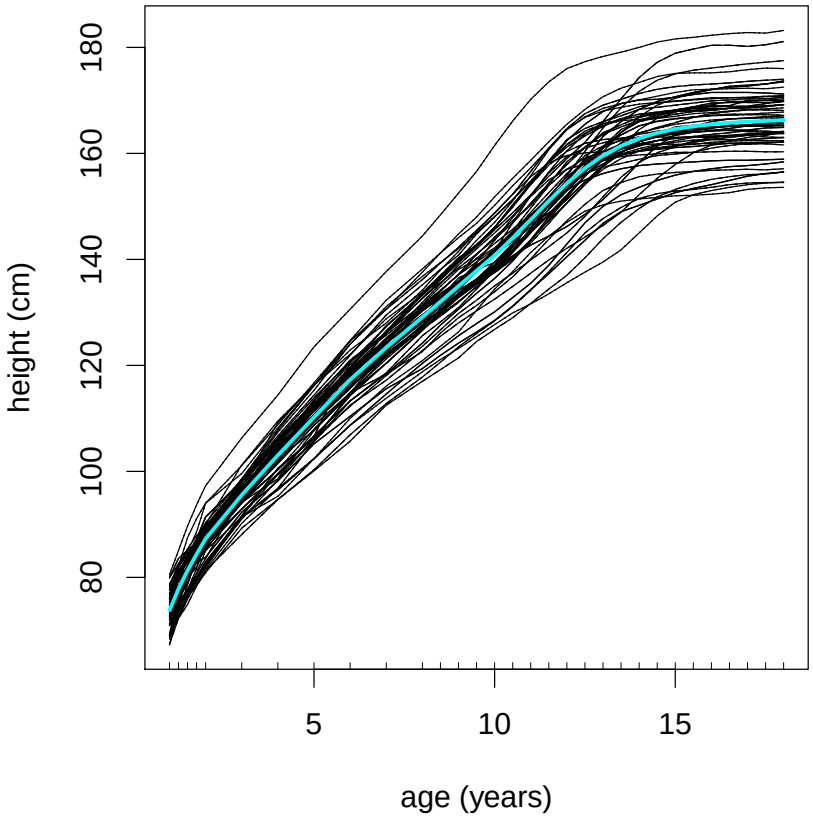
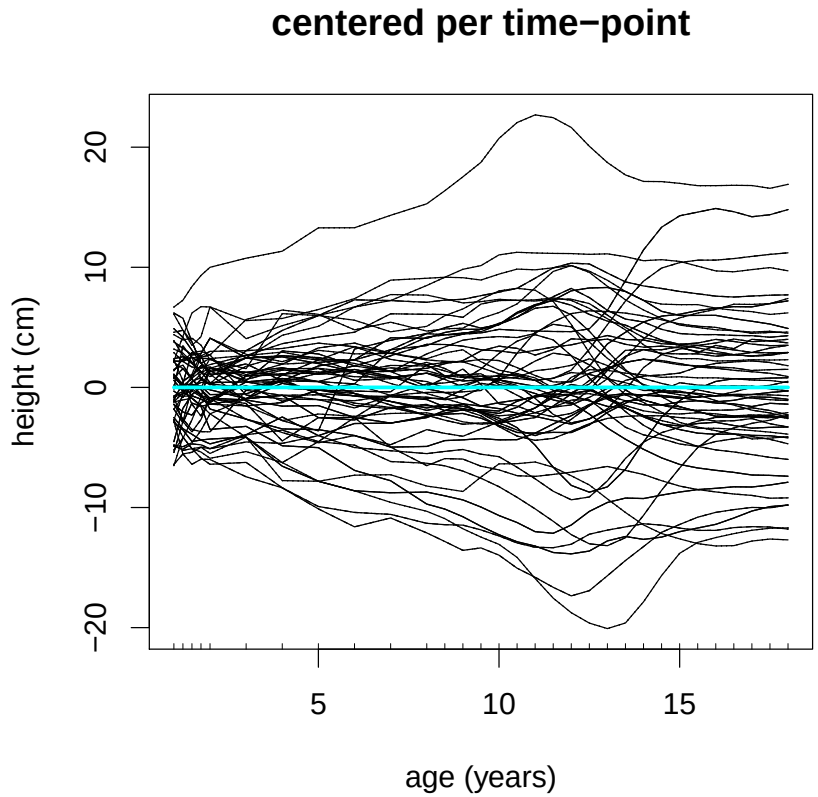
- functional (auto-)covariance:

$$\hat{\sigma}_X(t_1, t_2) = \frac{1}{n-1} \sum_{i=1}^{n} [x_i(t_1) - \bar{x}(t_1)][x_i(t_2) - \bar{x}(t_2)]$$

Example for mean: Growth curves of 54 girls





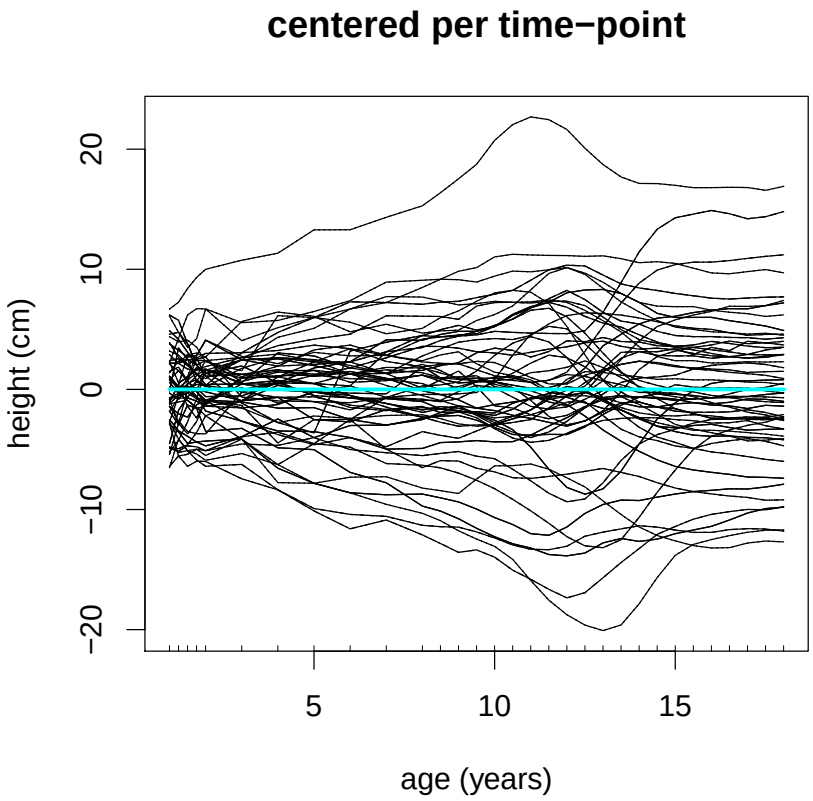
estimated mean:

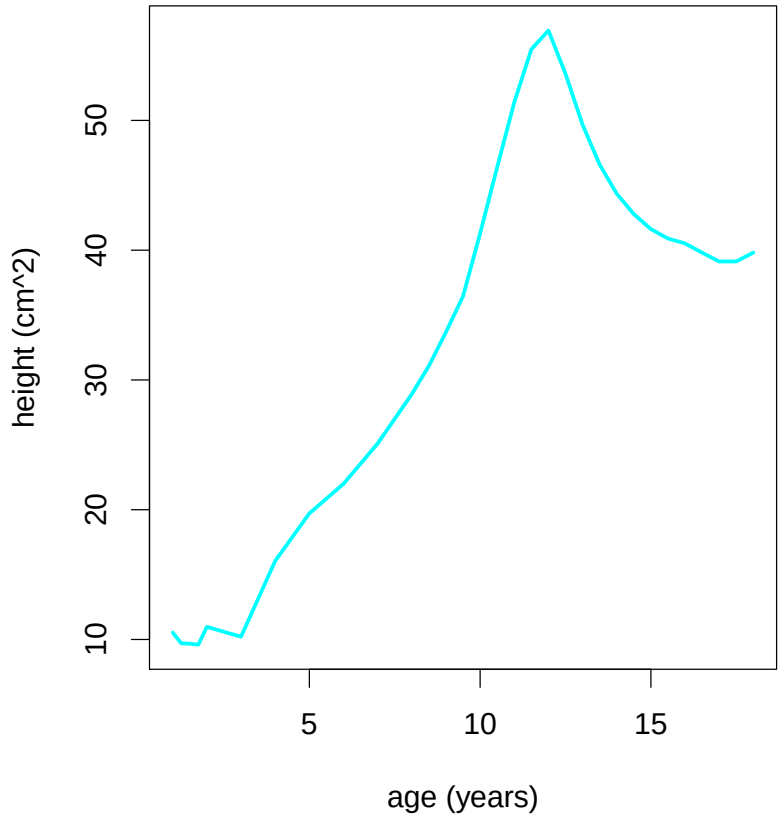
$$\hat{\mu}_X(t) = \bar{x}(t) = \frac{1}{n}\sum_{i=1}^{n} x_i(t)$$

centered curves:

$$x_i^*(t) = x_i(t) - \bar{x}(t)$$

Example for variance





centered curves:

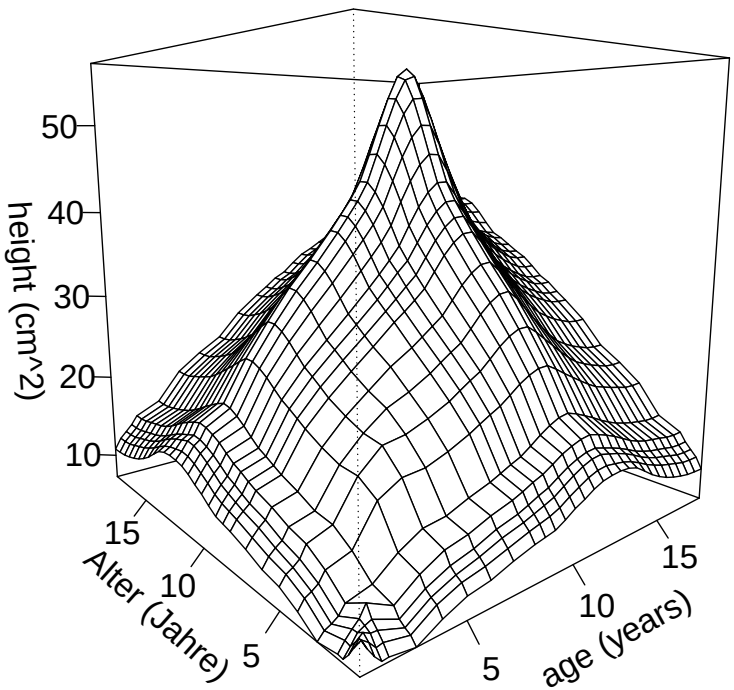
$$x_i^*(t) = x_i(t) - \bar{x}(t)$$

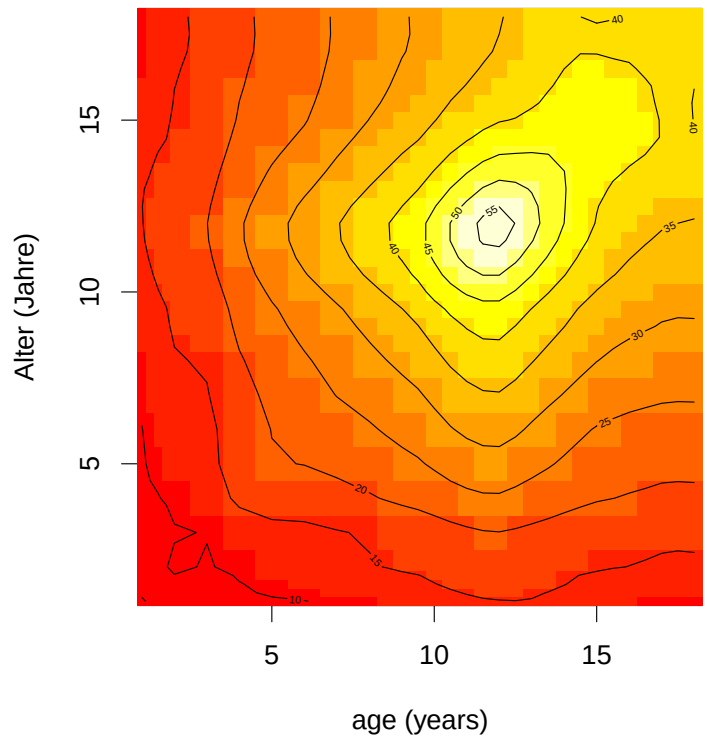
estimated variance:

$$\hat{\sigma}x(t) = \frac{1}{n-1}\sum_{i=1}^{n}[x_i(t) - \bar{x}(t)]^2$$

Example for covariance surface

$$\hat{\sigma}_X(t_1, t_2) = \frac{1}{n-1} \sum_{i=1}^{n} [x_i(t_1) - \bar{x}(t_1)][x_i(t_2) - \bar{x}(t_2)]$$





Outlook to functional data analysis

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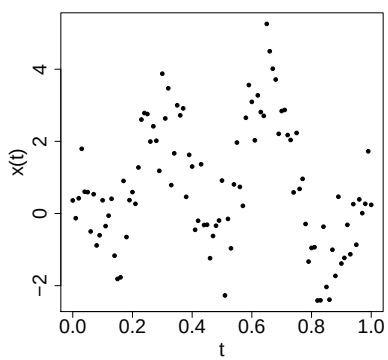
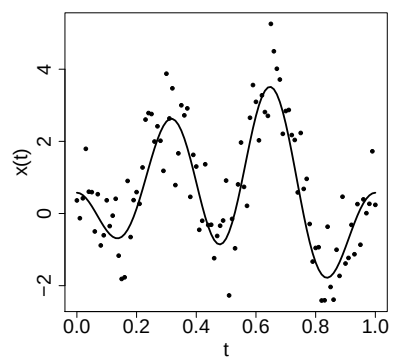
Important topics: (Ramsay & Silverman, 2005)

- Data representation $\rightarrow$ interpolation, smoothing





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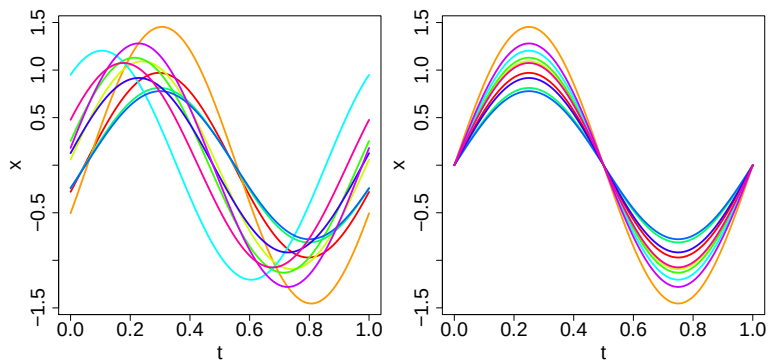

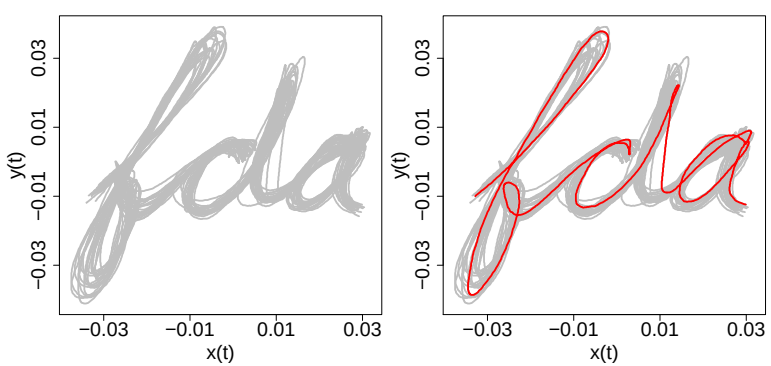

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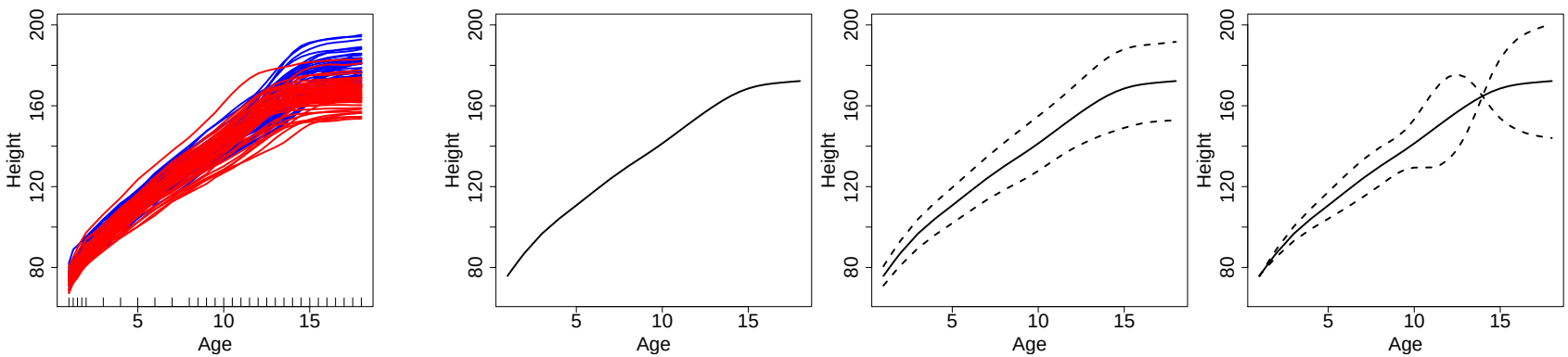
- Finding of patterns in the variation of the data $\rightarrow$ functional principal component analysis (FPCA)



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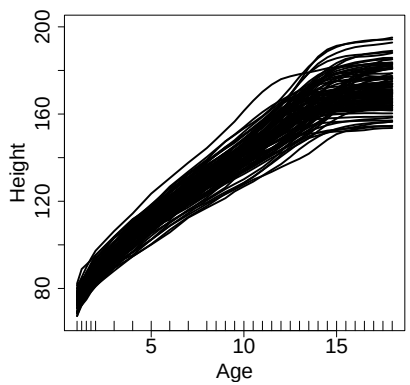

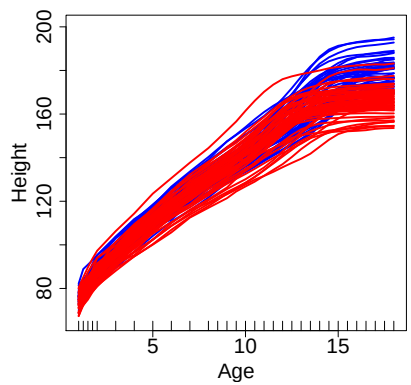

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- Classification and clustering
- Regression $\rightarrow$ functional regression models (Greven and Scheipl, 2017)

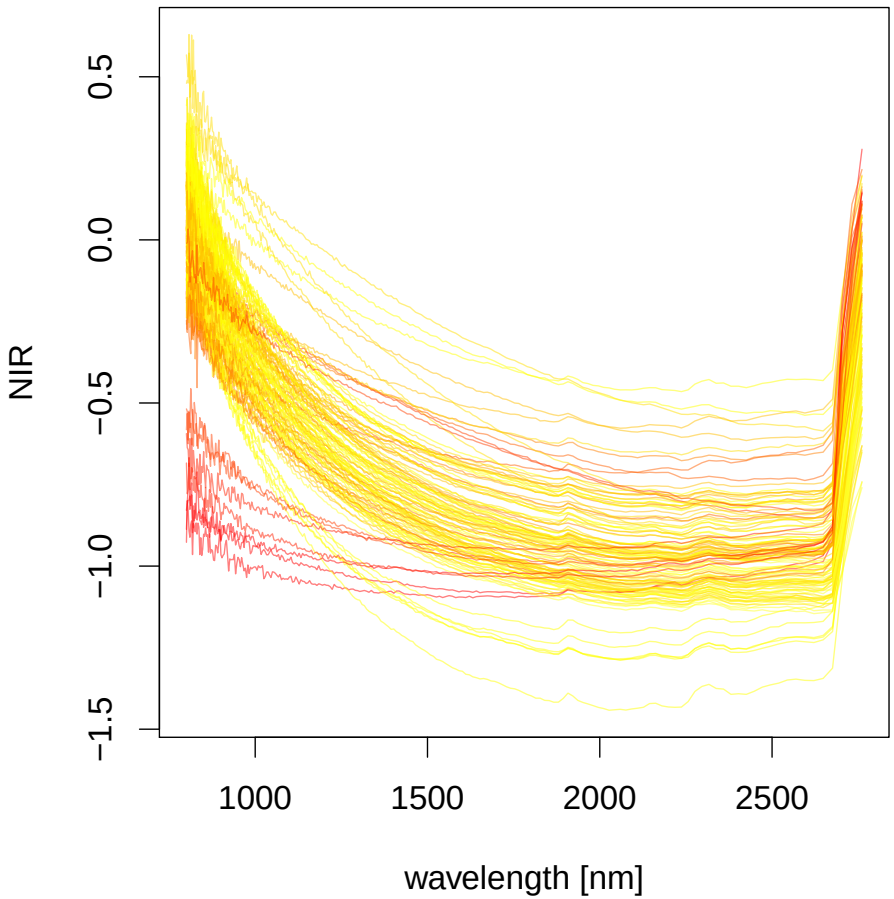
scalar-on-function: $$y_i = \mu + \int x_i(s)\beta(s)\mathrm{d}s + \varepsilon_i$$

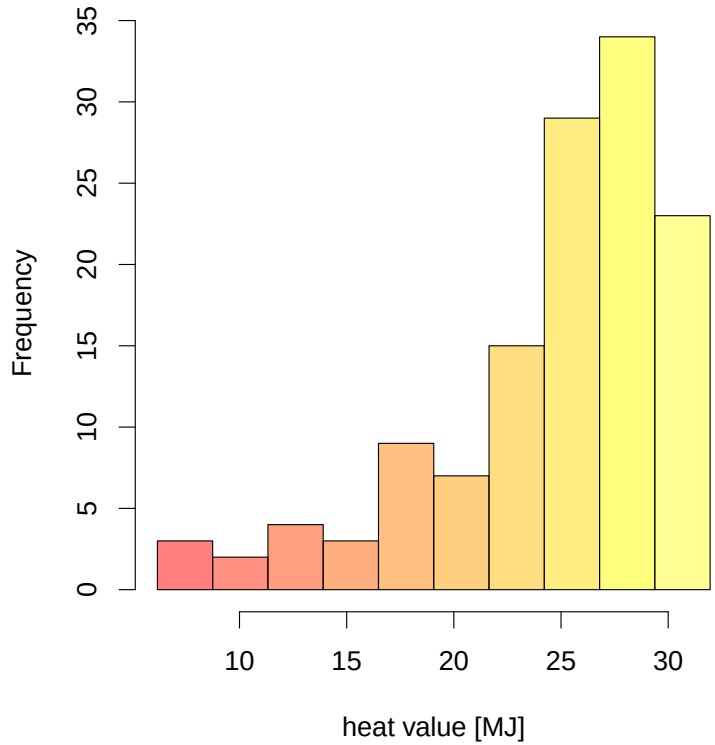
function-on-scalar: $$y_i(t) = \mu(t) + x_i\beta(t) + \varepsilon_i(t)$$

function-on-function: $$y_i(t) = \mu(t) + \int x_i(s)\beta(s,t)\mathrm{d}s + \varepsilon_i(t)$$

Spectral data of fossil fuels

aim: predict heat value y_i using the spectral measurement $x_i(s)$
Scalar-on-function-regression: $y_i = \mu + \int x_i(s)\beta(s)\mathrm{d}s + \varepsilon_i$





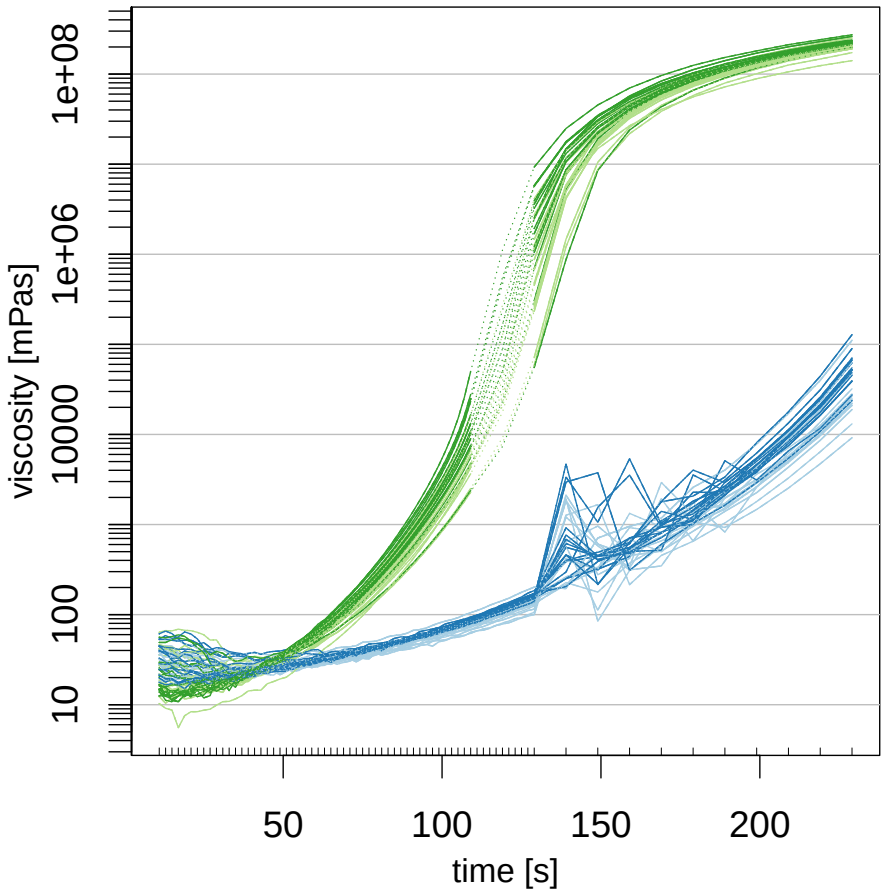
(Brockhaus et al. 2015)

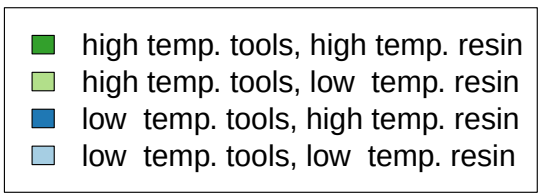
Viscosity of resin

aim: predict viscosity curve of resin depending on experimental conditions

Function-on-scalar-regression (functional ANOVA):

$$y_i(t) = \mu(t) + x_{i1}\beta_1(t) + x_{i2}\beta_2(t) + \varepsilon_i(t)$$



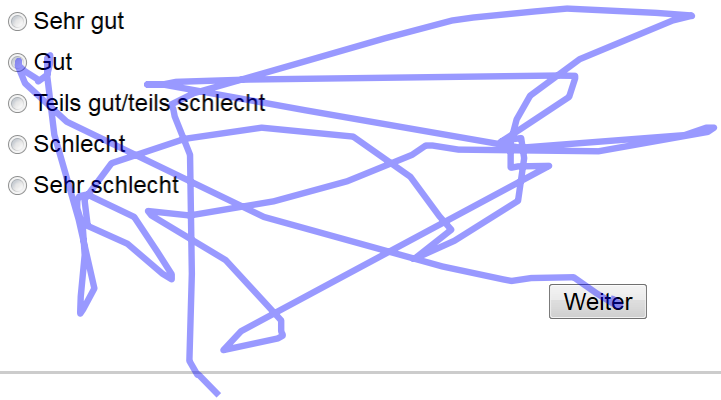


(Brockhaus et al. 2015)

Work in progress: Analysis of mouse cursor movements

Wie beurteilen Sie ganz allgemein die heutige wirtschaftliche Lage in Deutschland?

- Sehr gut
- Gut
- Teils gut/teils schlecht
- Schlecht
- Sehr schlecht



Weiter

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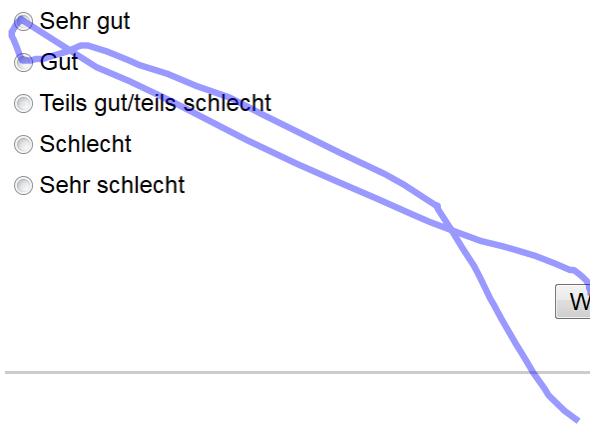

Weiter

Summary and discussion

- Measurement units are functions,
  i.e., curves, surfaces, trajectories,...
- Possibly arbitrary many measurements per function possible
  $\rightarrow$ Smooth data generating process
- Observations possibly with (measurement) error
- Many observations of the same data generating process

- Mean, variance and covariance for functional data
- Counterparts for many methods from multivariate statistics,
  like regression and classification with functional data

Literature and software

Literature and further reading

Monographs

- Ramsay & Silverman (2005), *Functional data analysis*, Springer, New York.
- Ferraty & Vieu (2006), *Nonparametric Functional Data Analysis*, Springer, New York

Overview articles

- Cuevas (2014), A partial overview of the theory of statistics with functional data, *Journal of Statistical Planning and Inference*, 147, 1–23.
- Levitin, Nuzzo, Vines & Ramsay (2007) Introduction to functional data analysis. *Canadian Psychology*, 48, 135–155.

Regression

- Greven & Scheipl (2017): A general framework for functional regression modelling. *Statistical Modelling*, to appear.
- Brockhaus, Scheipl, Hothorn & Greven (2015): The functional linear array model. *Statistical Modelling*, 15, 279–300.

R packages

Visualization

- Shang & Hyndman (2016). *rainbow: Rainbow Plots, Bagplots and Boxplots for Functional Data.* R package version 3.4. https://CRAN.R-project.org/package=rainbow

Visualization, descriptive and exploratory analysis

- Febrero-Bande & Oviedo de la Fuente (2012). *Statistical Computing in Functional Data Analysis: The R Package fda.usc.* Journal of Statistical Software, 51(4), 1–28.
- Ramsay, Wickham, Graves & Hooker (2014). *fda: Functional Data Analysis.* R package version 2.4.4. https://CRAN.R-project.org/package=fda

Regression

- Goldsmith, Scheipl, Huang, Wrobel, Gellar, Harezlak, McLean, Swihart, Xiao, Crainiceanu & Reiss (2016). *refund: Regression with Functional Data*. R package version 0.1-16. https://CRAN.R-project.org/package=refund